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# The MCNP Code: 6.3 and Beyond

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# Outline

Introduction

New Features

Future Work

# General Status of the MCNP Code

- ▶ There are a large number of new features and bugfixes relative to 6.2
- ▶ We are currently in the process of finalizing version 6.3 soon
- ▶ We are starting planning for 6.4 now

## New Features in 6.3

- ▶  $k$ -eigenvalue convergence improvements
- ▶ Doppler Broadening Resonance Correction (DBRC)
- ▶ FMESH performance and scaling improvements
- ▶ Better input and output formats
  - ▶ FMESH and EEOU: XDMF
  - ▶ Unstructured Mesh: HDF5
- ▶ Parallel PTRAC (with HDF5 output too)
- ▶ V&V infrastructure work
- ▶ General performance improvements
- ▶ And more.

# **k-eigenvalue Auto-convergence and Acceleration**

Added ability for MCNP to automatically detect convergence:

```
1 kcode 1000000 1.0 100 200
2 kopts fmat=yes fmataccel=yes fmatconvrg=yes
3      fmatsrc=yes fmatncyc=10
```

**fmat=yes** Enable fission matrix computation using same mesh as Shannon entropy.

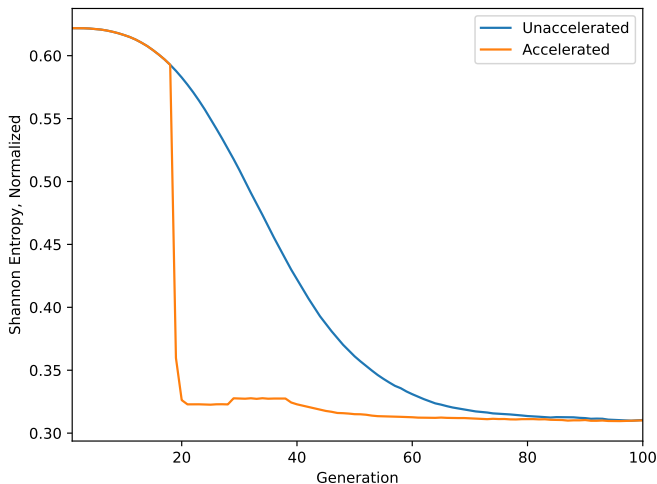
**fmataccel=yes** During inactive cycles, sample source distribution from fission matrix to accelerate convergence.

**fmatconvrg=yes** During inactive cycles, run 11 statistical tests to determine convergence. If tests pass, start active cycles.

**fmatsrc=yes** Start a uniform source in the mesh. Ideal for initial sampling of fission matrix.

**fmatncyc=10** Generations between solving the fission matrix.

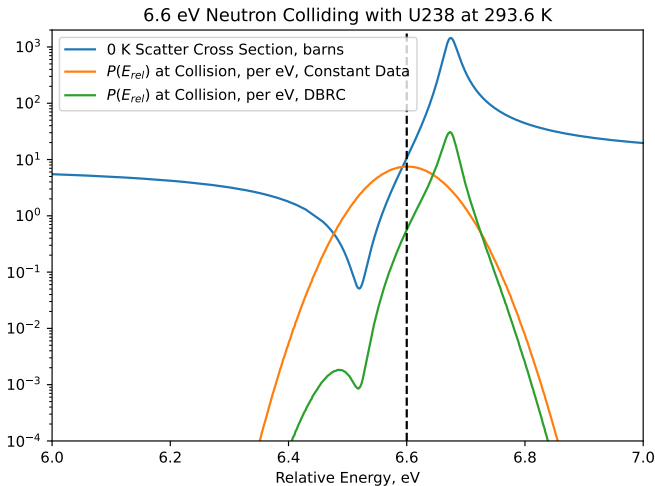
# $k$ -eigenvalue Auto-convergence and Acceleration



Test model is OECD Convergence Benchmark 4 (grid of 5x5 spheres, center larger).



# Doppler Broadening Resonance Correction (DBRC)



Before DBRC, integral scattering adjusted for Doppler broadening, but scattering kernel was not.

# Doppler Broadening Resonance Correction (DBRC)

Adding DBRC card enables corrections to the scattering kernel. Requires special 0 K nuclear data to be used.

```
1 dbrc endf=80
2      isos=[list of ZAIDs to apply DBRC, e.g. 92238]
```

Temperature	$k$ Before	$k$ After	$\delta k$ , pcm
293.6 K	$1.30580 \pm 0.00013$	$1.30531 \pm 0.00013$	$-49 \pm 18$
600 K	$1.28653 \pm 0.00013$	$1.28529 \pm 0.00013$	$-124 \pm 18$
2500 K	$1.20859 \pm 0.00013$	$1.20085 \pm 0.00012$	$-774 \pm 18$

For a PWR test problem. Usually insignificant at low temperatures, but can be important at high temperatures.

All cells must have TMP cards for this to work correctly. Data is preprocessed for ENDF/B-VII.1 and ENDF/B-VIII.0. The utility that did so will come with the code.

# FMESH Performance

Entire FMESH parallelism backend was replaced with a new one. Exposes the tally keyword-value option:

```
1 fmesh4:n tally={hist,fast_hist,batch,rma_batch}
```

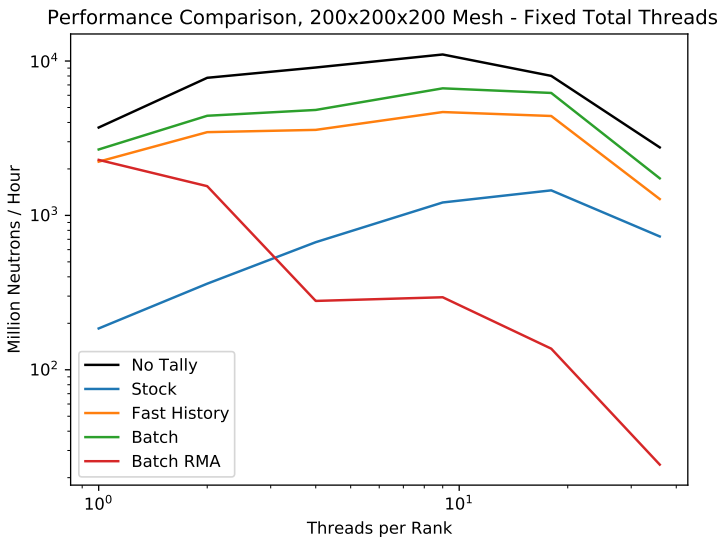
**hist** Basic history statistics tally.

**fast\_hist** Performance tuned history statistics tally. Default. Matches previous answers.

**batch** Performance tuned batch statistics tally.

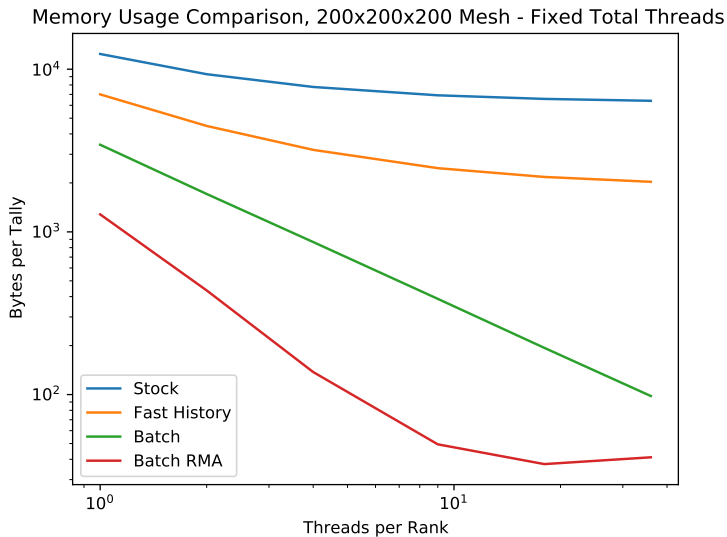
**rma\_batch** Remote memory access version of batch. For extremely large problems (think 10s of billions to trillions of tally zones). Distributes tallies over compute nodes.

# FMESH Performance



“Stock” results are from 6.2.

# FMESH Performance



# Output Files

We are generally moving towards XDMF + HDF5 for output, so as to be easily loaded into ParaView and other such tools.

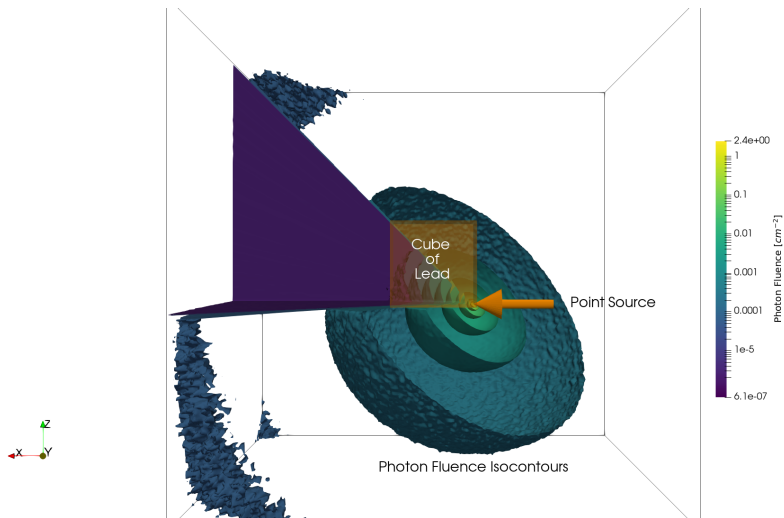
XDMF was chosen to minimize the number of dependencies for the MCNP code.

So far changed:

- FMESH tallies
- EEOUT tallies

More to come after 6.3.

# Output Files



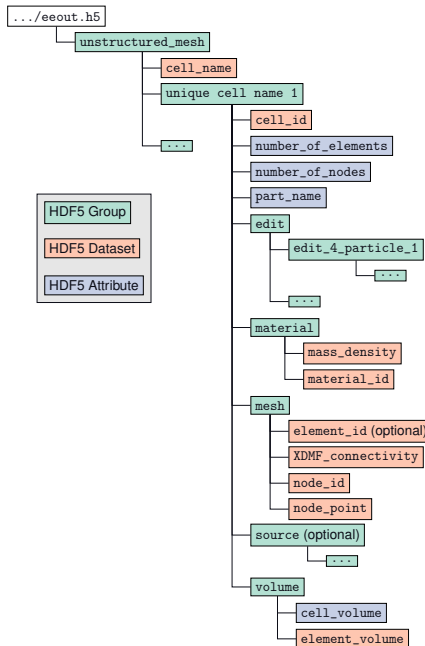
Neat plots like this (ParaView) are much easier with MCNP version 6.3.

# Unstructured Mesh Input/Output Format

- ▶ A relatively simple HDF5-based mesh format added to 6.3
- ▶ Alternative to current Abaqus format
- ▶ Documented in our manual
- ▶ Non-standard format, but other formats readily convertible to it
- ▶ Used in the same general way as formats in previous versions of the unstructured mesh capability



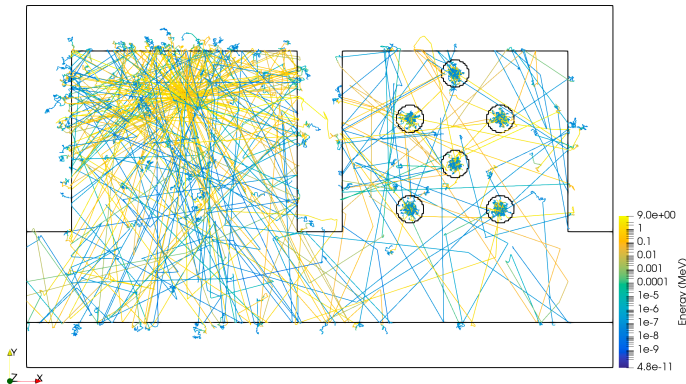
# Unstructured Mesh Input/Output Format



# Parallel PTRAC

- ▶ The PTRAC option can now be used with OpenMP or MPI
- ▶ Resulting file is in HDF5 format
- ▶ MCNPTools supports processing the HDF5 file in Python

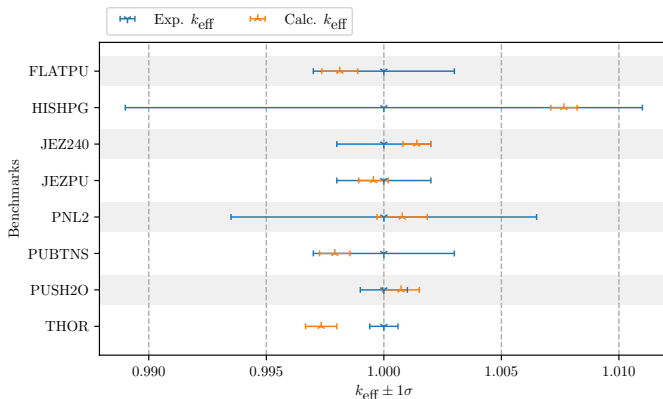
ParaView PTRAC visualization:



# V&V Infrastructure

The MCNP code has a lot of associated V&V. We are in the process of creating a unified framework to:

- ▶ Run models
- ▶ Compare them against experiment (via plotting, etc.)
- ▶ Compare against prior versions of the code



# Plans for the Future

Currently, our plans are very nascent for 6.4.

Work in progress:

- ▶ All TMESH features being added to FMESH
- ▶ Source plugin architecture (no recompiling for custom source routine)
- ▶ Delta tracking support
- ▶ Full ENDF/B-VIII.1 support

Work under consideration/planning:

- ▶ Implementing new tally backend everywhere
- ▶ Generalized tally sensitivity capability
- ▶ Energy deposition improvements
- ▶ Reducing or removing scaling limitations as feasible
- ▶ CADIS/FW-CADIS global variance reduction
- ▶ More HDF5 output options

## Questions?

Feel free to contact me at [cjosey@lanl.gov](mailto:cjosey@lanl.gov).